

Hexachlorophene
70-30-4 | DTXSID6020690

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 167 °C

Global applicability domain: Inside

Local applicability domain index: 4.89e-01

Confidence level: 6.47e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Hexachlorophene</div> <div>Measured: 167</div> <div>Predicted: 167</div>	<div>Image not found</div> <div>3,3',5,5'-Tetrabromobisphenol A</div> <div>Measured: 181</div> <div>Predicted: 174</div>	<div>Image not found</div> <div>Bithionol</div> <div>Measured: 188</div> <div>Predicted: 182</div>
<div>Image not found</div> <div>2,2',6,6'-Tetrachlorobisphenol A</div> <div>Measured: 135</div> <div>Predicted: 148</div>	<div>Image not found</div> <div>Fenticlor</div> <div>Measured: 174</div> <div>Predicted: 177</div>	